Simulation of the Radiative & Heterogeneous Chemical Impacts of Tropospheric Aerosol & Dust in the GMI Model

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Abstract

In this report, we give a description of the changes that were made to simulate the radiative and heterogeneous chemical impacts of aerosols on trace gas chemistry in the GMI code. The new coding additions are to the 1) tropospheric and combined tropospheric-stratospheric chemical mechanisms, involving the production of new setkin files, 2) the modification of fastj and some input files, and the 3) write-up of new routines for computations as well as for I/O.

1 Introduction

Aerosols play important roles in global climate change. They affect the earth's radiative budget by scattering or absorbing radiation and by altering cloud properties. The magnitude of these effects, however, is poorly constrained, because we have a limited knowledge of the processes that control the distributions as well as the physical, chemical, and optical properties of aerosols.

Understanding the radiative and heterogeneous chemical effects of aerosols on OH and O_3 , the main tropospheric oxidants, is a major issue for models of the oxidizing power of the atmosphere, radiative forcing, and surface air quality. Including photochemical effects of aerosols in global models could help resolve some long-standing discrepancies with measurements.

We include in the GMI code [2] the following major tropospheric aerosol types: sulfate, dust, organic carbon (OC), black carbon (BC), and sea salt aerosols. We use global distributions of aerosols from the GOCART model to estimate their optical depths and surface areas for use in the radiative and heterogeneous chemical portions of the code.

We report here the changes that were made in the GMI code to accomplised this task. The assessment of the new implementation will be done by verifying how it can reproduce the plots of column mass and optical depth for different aerosols and dust as presented in [1, 3].

This document is organized as follows. Section 2 provides the steps employed for incorporating aerosol/dust computation in the GMI code. Numerical experiments used to validate the new implementation are described in Section 3 and some conclusions are formulated in Section 4. Appendix A provides the aerosol/dust-related diagnostics added whereas Appendix B presents the new namelist variables, gives the input files needed to execute the code and points to the location of output files resulting from simulations done in this study. In Appendix C, we report all the changes made in the code.

2 Procedures

Our implementation of these processes closely follows the one done in GEOS-CHEM. We initially adapted to the GMI code the two GEOS-CHEM routines, RDAER and RDUST. The corresponding GMI routines are:

Aero_OptDep_SurfArea: Calculates optical depth at each level for the routine "Control_Fastj". It also calculates surface area for heterogeneous chemistry. It uses aerosol parameters in FAST-J input file "jv_spec.dat" for these calculations.

Dust_OptDep_SurfArea: Calculates dust optical depth at each level for the FAST-J routine "Control_Fastj". It uses dust parameters in FAST-J input file "jv_spec.dat" for these calculations.

Unlike GEOS-CHEM, the reading of the global aerosol and mineral dust concentrations (as determined by M. Chin and P. Ginoux) is done in a routine called *Read_Aerosol_Dust*. The reason is that for GMI the concentrations are available in a unique file and the reading is done by the master processor only.

The aerosol fields are provided by Mian Chin and the code from Randall Martin. One important modification to Martin's implementation [3] is that the reaction probability (i.e., sticking coefficient) for N_2O_5 is now a function of aerosol type, relative humidity, and temperature (Mat Evans, personal communication).

The original GMI code from LLNL treated heterogeneous chemical loss on sulfate aerosols, though only by uptake through molecular collisions. For a more comprehensive treatment and following GEOS-CHEM, we include now uptake by gas phase diffusion to the aerosol surface:

```
FRH = relative humidity fraction (0-1)

ntotA = number dust bins + number other aerosol bins

radA = radius of aerosol (cm)

ad = molec/cm^3 air

tk = temperature (K)

sad = surface area of aerosols/volume of air (cm^2/cm^3).
```

The loss rate (k = 1/s) of species on aerosol surfaces is given by

$$k = sad \times \left[\frac{radA}{Dq} + \frac{4}{v\gamma}\right]^{-1},$$

where

 $Dg = \text{gas phase diffusion coefficient}(cm^2/s)$

 γ = sticking coefficient or reaction probability (unitless)

 $v = \text{mean molecular speed } (cm/s) = \left[\frac{8RT}{pi \times M}\right]^{1/2}$ $\frac{radA}{Dg} = \text{uptake by gas-phase diffusion to the particle surface}$ $\frac{4}{v\gamma} = \text{uptake by free molecular collisions of gas molecules with the surface.}$

Remark 1 These code modifications were implemented for the GMI Tropospheric and Combo models.

3 Basic Experiments

A number of sensitivity simulations were done to:

- 1. Compare our results with those of Martin et al. [3] for evaluation purposes and
- 2. Gauge the model's response to the new aerosols.

We carried out four set of one-year experiments distinguished by whether radiative effects or/and heterogeneous chemistry on different aerosols/dust are turned off or/and turned on (see Appendix B):

Experiment 1 $AerDust_Effect_opt = 0$

Experiment 2 $AerDust_Effect_opt = 1$

Experiment 3 $AerDust_Effect_opt = 2$

Experiment 4 $AerDust_Effect_opt = 3$.

We present here a brief summary of our findings.

The net impact of simulating the heterogeneous chemical and radiative impacts of the aerosols is to decrease OH, O_3 , and NO_x by 13%, 6%, and 26%, respectively. The decrease in OH when weighted to reaction with methane is 16%. The methyl chloroform lifetime increases from 5.2 to 6.1 yrs and the mean tropospheric OH decreases from 1.1 to 0.95×10^6 $molec/cm^3$. These calculations were done using simulations with the effects of aerosols turned completely on or completely off.

The heterogeneous chemical impacts of all aerosols decrease OH, O_3 , and NO_x by 9%, 7%, and 29%, respectively, and the radiative impacts by 4%, 0%, and -1%, respectively.

A big contributor to the total impact of aerosols is N_2O_5 hydrolysis. However, with the implementation of the probability of reaction per collision as a function of aerosol type, relative humidity, and temperature, N_2O_5 hydrolysis is less important than when it is fixed equal to 0.1, as done previously in the GMI model. For instance, in a simulation with the probability equal to 0.1, OH, O3, and NO_x decrease by 20%, 11%, and 37%, respectively, which is a greater decrease than when the probability varies as shown above.

The heterogeneous chemical and radiative impacts of dust alone decrease OH, O3, and NO_x by 5%, 1%, and 5%, respectively. The weighted OH decrease is 6%. This percent decrease is lower than that presented in [3], which was 9%. There are several differences between our two models, so the individual model responses should be different. Some important differences are that the two models use different sulfate fields, absorption cross-sections, and probability of reaction per collision for N_2O_5 hydrolysis, etc. When we use the same probability of reaction, OH, O3, and NO_x decrease by 10%, 5%, and 18%, respectively. The weighted OH difference is 12%, which is now higher than the 9% reported by Martin et al. [3].

What is the impact of the new aerosol implementation as compared to the old one in the GMI model? We estimate that the old implementation (i.e., heterogeneous chemistry on sulfate with a probability of reaction equal to 0.1 for N_2O_5 hydrolysis) decreases OH, O3, and NO_x by 7%, 6%, and 27%, respectively. The new implementation decreases OH, O3, and NO_x by an additional 6%, 0%, and -1%, respectively. Though these percent decreases are quite large, the regional impacts of the new aerosol implementation are sometimes larger, especially over the Sahara Desert, India, and tropical regions that are experiencing biomass burning.

4 Conclusion

We described how aerosol and mineral dust computations were incorporated in the Tropospheric and Combo chemical mechanism of the GMI code. The new additions were fully tested and verified to produce results similar to the ones appearing in the literature. We plan to make the aerosol code compatible with Fast-Jx.

References

- [1] M. Chin et al., Tropospheric aerosol optical thickness from the GOCART model and comparisons with satellite and sun photometer measurements, *J. Atmos. Sc.*, **59**, p. 461–483, (2002).
- [2] J. Kouatchou, В. Das Η. Oloso. GlobalModeling and Inititutorialanduser'squide, online documentation available http://gmi.gsfc.nasa.gov/tutorial/index.html.
- [3] R.V. Martin, D.J. Jacob, R.M. Yantosca, M. Chin, and P. Ginoux, Global and regional decreases in tropospheric oxidants from photochemical effects of aerosols, em J. Geo. Res., 108(D3), doi:10.1029/2002JD002622, (2003).

A New Diagnostics

The following monthly average diagnostics (optical depth, surface area and column mass for various aerosols/dust) were added:

```
Cloud optical depths (1000 nm)
Max Overlap Cloud Fraction
Random Overlap Cloud Fraction
Dust optical depths (400 nm)
Dust surface areas
Sulfate Optical Depth (400 nm)
Hygroscopic growth of SO4
Sulfate Surface Area
Black Carbon Optical Depth (400 nm)
Hygroscopic growth of Black Carbon
Black Carbon Surface Area
Organic Carbon Optical Depth (400 nm)
Hygroscopic growth of Organic Carbon
Organic Carbon Surface Area
Sea Salt (accum) Opt Depth (400 nm)
Hygroscopic growth of Sea Salt (accum)
Sea Salt (accum) Surface Area
Sea Salt (coarse) Opt Depth(400 nm)
Hygroscopic growth of Sea Salt (coarse)
Sea Salt (coarse) Surface Area \\
Dust Column Mass (g/m2)
Sulfate Column Mass (g/m2)
Black Carbon Column Mass (g/m2)
Organic Carbon Column Mass (g/m2)
```

These diagnostics are contained in the new file < problem_name >.AerDust.nc.

B Namelist Variables and Input/Output Files

Three namelist variables were included in the code:

Sea Salt Column Mass (g/m2)

1. AerDust_Effect_opt: Choose if the radiative effects or/and heterogeneous chemistry on different aerosols/dust are turned on/off.

```
=0: radiative effects on and heterogeneous chemistry on=1: radiative effects off and heterogeneous chemistry on=2: radiative effects on and heterogeneous chemistry off=3: radiative effects off and heterogeneous chemistry off
```

- 2. AerDust_infile_name: global aerosol and mineral dust concentrations input file name
- 3. *pr_AerDust*: should the periodic aerosol/dust diagnostics be written?

An example of setting (for Experiment 1) of the new namelist variables is:

```
&ACTM_INPUT
    .
    .
    .
    .
    AerDust_Effect_opt = 0,
    AerDust_infile_name = 'aerosol_dao_Y1997.nc' /
&ACTM_OUTPUT
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    .
    .
    pr_AerDust = T,
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```

The following input files were needed for the runs:

uvalbedo.geos.4x5.ascii

```
DAO_GS_4x5x46.in
                                   : listing of met field files
fixed_ACET_CH4_gmi_dao_4x5.nc
                                 : fixed const.
aerosol_dao_Y1997.nc
                                   : global aerosol and mineral dust
                                     concentrations
gmit4_dao_dec_withoutMNO3_dec.rst.nc: restart
gmi_DAO4x5_020731.nc
                                  : emissions
vegtype_4x5_dao.asc
                                   : vegetation type
lai_4x5_dao.asc
                                  : leaf area index
DAO_gmit3_sad.nc
                                  : liquid binary sulfate
                                   : modified cross section
AerDust_jv_spec.dat
AerDust_ratj.d
                                  : modified rate
jv_atms.dat
                                   : climatology
```

Output files for the experiments described in Section 3 are available on *dirac* in the respective directories:

: Uv albedo

```
pub/gmidata/gmit/AerDust_Test/gmta_dao_AerDustAllOn_Y0201-0212_1
pub/gmidata/gmit/AerDust_Test/gmta_dao_AerDustNoRadiative_Y0201-0212_1
pub/gmidata/gmit/AerDust_Test/gmta_dao_AerDustNoHetero_Y0201-0212_1
pub/gmidata/gmit/AerDust_Test/gmta_dao_AerDustAllOff_Y0201-0212_1
```

C List of Changes

We list all the changes that were introduced in the code. In particular, we report the variables that were added and the files and routines affected by the additions.

C.1 Changes Inside the Code

```
include/
  gem_msg_numbers.h
     For sub domains to global domain
       ACTM\_SG\_OptDepth\_NC = 272
       ACTM_SG_CM_AerDust = 273
       ACTM_SG_GridHeight = 274
     For global domain to sub domains
       ACTM_DAERSL(2) = (/ 810, 811 /)
       ACTM_WAERSL(5) = (/ 820, 821, 822, 823, 824 /)
       ACTM_DUST(7) = (/ 830, 831, 832, 833, 834, 835, 836 /)
  gem_config.h
     Add "-lACTMAerosol_Dust" to the list of libraries ACTMLibs.
actm/gmimod/include/
  gmi_control.h
     AerDust_Effect_opt : Choose if the radiative effects or/and
                          heterogeneous chemistry on different
```

heterogeneous chemistry on different
aerosols/dust are turned on/off.

=0: radiative effects on and heterogeneous chemistry on
=1: radiative effects off and heterogeneous chemistry on

=1: radiative effects off and heterogeneous chemistry on =2: radiative effects on and heterogeneous chemistry off =3: radiative effects off and heterogeneous chemistry off

gmi_arrays_out_mas_sl.h
 OptDepth_nc

gmi_gen_io.h

num_AerDust = 20 : Number of entries for aerosol/dust diagnostics

num_CM_AerDust= 5 : Number of column mass entries for aerosol/dust diagnostics

AerDust_var_name : NetCDF aerosol/dust variable name ncid_AerDust : NetCDF aerosol/dust output file id rnum_out_AerDust : next aerosol/dust record to writ

AerDust_infile_name: global aerosol and mineral dust concentrations input

file name

AerDust_labels : labels for aerosol/dust diagnostics

CMAerDust_labels : labels for aerosol/dust column mass diagnostics

pr_AerDust : should the periodic aerosol/dust diagnostics be written?

```
New files:
    gmi_AerDust_calc.h contains variables used for calculations
        OptDepth : Optical Depth and surface area diagnostics
        ERADIUS
                   : Aerosol or dust radii [cm]
        TAREA
                  : Surface area of aerosol or dust [cm2/cm3]
                  : Relative humidity [H2O molec/cm3]
        REL_HUM
        ODAER
                  : Optical depth for aerosol
        ODMDUST : Optical for mineral dust
        ColMassDust : Dust
                                   Column Mass (g/m2)
        ColMassSO4 : Sulfate
                                  Column Mass (g/m2)
        ColMassBC : Black Carbon Column Mass (g/m2)
        ColMassOC : Organic Carbon Column Mass (g/m2)
        ColMassSS : Sea Salt
                                  Column Mass (g/m2)
    gmi_AerDust_const.h contains constant variables
               = 5 : number of relative humidity bins
        nrh_b
        NP_b
               = 56
    gmi_AerDust_input.h contains variables used for input only
                 : Mass density of hydrophobic aerosol (kg/m3)
        WAERSL
                 : Mass density of hydrophilic aerosol (kg/m3)
        DUST
                : Mass density of Dust
                : Aerosol scattering phase functions
        QAA_b
                 : Effective radius associated with aerosol type
        RAA_b
actm/gmimod/in_out
 gmi_netcdf_out_init.F
    Introduce the new routine Define_Netcdf_Out_AerDust.
 gmi_netcdf_out_write.F
    Introduce the new routine Write_Netcdf_AerDust.
    In Write_Netcdf_Nc, call Write_Netcdf_AerDust.
 gmi_netcdf_out_prep.F
    Introduce the new routine Prep_Netcdf_AerDust.
    In Prep_Netcdf_Nc, call Prep_Netcdf_AerDust.
 gmi_netcdf_out_wrthd.F
    Introduce the new routine Write_Netcdf_Hdr_AerDust.
 gmi namelist.F
    Add the variables: AerDust_var_name, AerDust_infile_name, pr_AerDust
actm/gmimod/aerosol_dust/
 This is a new directory containing the files:
    - gmi_calc_AerDust_ColumnMass.F
      Computes column mass for aerosols/dust.
    - gmi_calc_AerDust_odsa.F
      Computes optical depth and surface area for aerosols/dust.
```

- gmi_read_AerDust.F
 Reads (by the master processor) the monthly average aerosol
 file
- gmi_set_AerDust_labels.F
 Sets the aerosol/dust labels needed for output.
- my_Read_TJPL.F
 Reads the cross section file to extract the variables
 QAA_b and RAA_b needed to compute optical depth and surface area

actm/gmimod/control/

actm_adv_output.F

In the routine Control_Nc_Output, update the value of "rnum_out_AerDust" to move to the next record to be written out in the AerDust output file. Also set values of OptDepth, ColMassDust, ColMassSO4, ColMassBC, ColMassSC, ColMassSC to zero after they are written out in the file.

actm_advance.F

Call (in Do_Oneproc_Adv and Do_Multiproc_Adv) the routine Reading_Aerosol_Dust to allow the master processor to read aerosol/dust data.

Call (in Do_Multiproc_Adv) the routine AerDust_Glob_To_Sub to send aerosol/dust data to the slave processors.

actm/gmimod/mem_manage/

gmi_alloc.F

Allocate the variables contained in the include files gmi_AerDust_calc.h and gmi_AerDust_input.h

actm/gmimod/comm/

gmi_buffer.F

Introduce the new routine Buffer_Output_AerDust and call it in Buffer_Output_Nc.

gmi_sub_to_glob.F

Introduce the new routine Sub_To_Glob_Aer and call it in Sub_To_Glob_Nc.

gmi_glob_to_sub.F

Introduce the new routine AerDust_Glob_to_Sub.

$\operatorname{actm/gmimod/step}/$

qj_update.F

Compute in the routine Update_Qj:

- the column mass (routine AerDust_ColumnMass) for

```
aerosols/dust.
```

- the optical depth and surface area (routine Aero_OptDep_SurfArea) for aerosols.
- the optical depth and surface area (routine Dust_OptDep_SurfArea) for dust.

Pass on the values of optical depht (ODAER_ij, ODMDUST_ij) aerosols/dust to the fastj control routine.

qk_update.F

In the Update_Qk, add the variables "sadcol2", "radA" (surface area) and "rhcol" (relative humidity column) that are arguments of the routine Kcalc. The three variables are calculated before they are passed to Kcalc.

actm/gmimod/phot/fastj/

newcol.F

In the routine set_prof, rewrite the section on "Add Aerosol Column".

In the routine set_aer, add more values to the array MIEDX (index 4 to 35) aerosol/dust species.

fastj_control.F

In the routine Control_Fastj:

- add "ODAER_ij" and "ODMDUST_ij" as arguments to Control_Fastj.
- assign ODAER_ij to "optaer" and "ODMDUST_ij" to "optdust".

${\bf actm/gmimod/chem/troposphere}$

New setkin files (with only 85 species: MNO3 or MeNO3 was removed).

setkin_par.h

NSADdust : number of dust bins NSADaer : number of other aerosol bins

C.2 Changes in the Input Files

- The cross section input file (jv_spec.dat) was modified to add information on aerosols/dust. The section on "aerosol phase functions" now contains 56 subdivisions instead of 14.
- The rate input file (ratj.d) was modified to remove the line referring to MeNO3. The indices on the first column were reajusted accordingly.
- The restart file (needed to start the run for the first time) was modified to take into account the reduction of the number of species.
- The input file containing information on aerosols/dust at various bins was added. It is passed through the namelist variable "AerDust_infile_name".